Convex Multilinear Estimation and Operatorial Representations

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Outline

Convex Multilinear Estimation

Preliminaries

Learning with Sparsifying Penalties: from Vectors to Tensors

CMLE: A First Order Algorithm

Learning the Tensor with CMLE

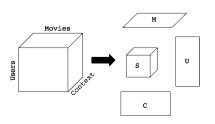
Unsupervised Learning Supervised Learning

Beyond Linearity: Tensors and Kernels

A Framework for Non-parametric Tensor-based Models Experiments

Tensor-based Models: A Machine Learning Perspective

- Tensors are tricky to deal with: non-convex problems
- Exploit the intrinsic structure of data: multiple views
- Leads to linear models: limited discriminative power!
- Very effective for small sample problems

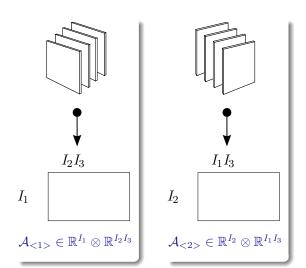


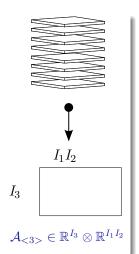
One could argue that the most important aspect of intelligence [...] is the ability to learn from very few examples. [...] Evolution has probably done a part of the learning but so have we, when we choose for any given task an appropriate input representation for our learning machines.

The Mathematics of Learning: Dealing with Data T. Poggio and S. Smale

n-mode Unfolding $\mathcal{A}_{\leq n \geq}$ of a Tensor \mathcal{A}

 $\mathcal{A} \in \mathbb{R}^{I_1} \otimes \mathbb{R}^{I_2} \otimes \mathbb{R}^{I_3}$. Unfolding = concatenation of slices





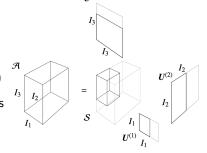
Multilinear Singular Value Decomposition (MLSVD)

Matrix SVD:
$$m{A} = \sum_{i=1}^{\min\{I_1,I_2\}} \sigma_i U_i V_i^{ op} = m{U} m{S} m{V}^{ op} = m{S} imes_1 m{U} imes_2 m{V}$$

Higher Order Extension: the Third Order Case

$$\mathcal{A} = \mathcal{S} \times_1 \mathbf{U}^{(1)} \times_2 \mathbf{U}^{(2)} \times_3 \mathbf{U}^{(3)}$$

- \triangleright S is the core tensor (same size as A)
- $m U^{(1)}, m U^{(2)}, m U^{(3)}$ orthogonal matrices
- ightharpoonup \equiv SVD's of the n-mode unfoldings
- notion of multilinear ranks



Truncated MLSVD leads to low multilinear ranks approximation

A Convex Approach to Tensor-based Data Analysis

Goal

Develop a general approach to tensor-based modeling via convex optimization

We go through three steps:

- 1. Sparsity Inducing Penalties: from Vectors to Higher Order Tensors
- 2. General Convex Formulation
- 3. Viable Algorithm

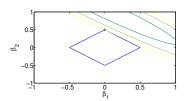
Learning by Penalized Empirical Risk Minimization

$$\hat{W} = \arg\min_{W \in \mathbb{R}^{I}} \left\{ J(W) + \lambda r(W) \right\}$$

- ightharpoonup J(W) measures model fit to the data (depends on the task)
- ightharpoonup r(W) is a penalty function

Sparsity inducing penalty: l_1 Norm of $W \in \mathbb{R}^I$

$$r(W) = ||W||_1 = \sum_{i=1}^{I} |w_i|$$



▶ Best convex approximation of $card(W) = \#\{i : w_i \neq 0\}$

Nuclear Norms: from Matrices to Tensors

$$r(\mathbf{\textit{W}}) = \|\mathbf{\textit{W}}\|_1 = \sum_{i=1}^{\min\{I_1,I_2\}} \sigma_i = \|\sigma\|_1, \ \mathbf{\textit{W}} = \sum_{i=1}^{\min\{I_1,I_2\}} \sigma_i \, U_i \, V_i^\top \ .$$

▶ Best convex approximation of rank(\mathbf{W}) = $\#\{i : \sigma_i \neq 0\}$

Higher Order Generalization of the Nuclear Norm

$$\begin{array}{ccc} \text{Matrices} & \text{Tensors of Order N} \\ & \to & \\ \| \, \boldsymbol{W} \|_1 = \sum_{i=1}^{\min\{I_1,I_2\}} \sigma_i & \| \mathcal{W} \|_{1,1} = \frac{1}{N} \sum_{n=1}^N \| \mathcal{W}_{< n>} \|_1 \end{array}$$

 $\|\mathcal{W}\|_{1,1}$ penalizes high multi-linear ranks (related to the MLSSVD)

A class of Optimization Problems Involving Nuclear Norms

$$\begin{aligned} \min_{\mathcal{W} \in \mathbb{R}^{I_1} \otimes \mathbb{R}^{I_2} \otimes \cdots \otimes \mathbb{R}^{I_N}} \quad & J(\mathcal{W}) + \lambda \|\mathcal{W}\|_{1,1} \\ \text{subject to} \quad & A(\mathcal{W}) = \mathcal{Z} \end{aligned}$$

- lacktriangle convex and smooth function $J:\mathbb{R}^{I_1}\otimes\mathbb{R}^{I_2}\otimes\cdots\otimes\mathbb{R}^{I_N}\to\mathbb{R}$
- $lacktriangleright \lambda > 0$ is a user-defined regularization parameter
- A is a linear transformation

Different choices of J and A give rise to different problems

Convex MultiLinear Estimation (CMLE) Algorithm

$$\begin{array}{l} \textbf{input } \mathcal{W}^{(0)}, \text{ dual variables } \boldsymbol{P}^{(0)}_{(1)}, \dots, \boldsymbol{P}^{(0)}_{(N)}, \mu, c \\ k \leftarrow 1 \\ \mathcal{W}^{(k)} \leftarrow \mathcal{W}^{(0)} \\ \boldsymbol{P}^{(k)}_{(n)} \leftarrow \boldsymbol{P}^{(0)}_{(n)} \\ \textbf{repeat} \\ \\ \mathcal{S} \leftarrow \nabla J(\mathcal{W}^{(k)}) \leftarrow \boxed{\text{gradient of the problem-dependent part}} \\ \textbf{for } n \in \mathbb{N}_N \textbf{ do} \\ \\ \boldsymbol{W}^{(k+1)}_{(n)} \leftarrow D_{\frac{\mu}{c}} \left(\mathcal{W}^{(k)}_{< n>} - \frac{1}{c} \mathcal{S}_{< n>} + \frac{1}{c} \boldsymbol{P}^{(k)}_{(n)} \right) \leftarrow \boxed{\text{singular values}} \\ \boldsymbol{P}^{(k+1)}_{(n)} \leftarrow \boldsymbol{P}^{(k)}_{(n)} + c \left(\mathcal{W}^{(k)}_{< n>} - \boldsymbol{W}^{(k+1)}_{(n)} \right) \\ \textbf{end} \\ \mathcal{W}^{(k+1)} \leftarrow \frac{1}{N} \sum_{n \in \mathbb{N}_N} \left(\boldsymbol{W}^{(k+1)}_{(n)} - \frac{1}{c} \boldsymbol{P}^{(k+1)}_{(n)} \right)^{< n>} \\ \textbf{until convergence criterion met} \end{array}$$

Convexity implies global optimality of the solution found!

Supervised and Unsupervised Learning with CMLE

$$\begin{aligned} \min_{\mathcal{W} \in \mathbb{R}^{I_1} \otimes \mathbb{R}^{I_2} \otimes \cdots \otimes \mathbb{R}^{I_N}} \quad & J(\mathcal{W}) + \mu \|\mathcal{W}\|_{1,1} \\ \text{subject to} \quad & A(\mathcal{W}) = \mathcal{Z} \end{aligned}$$

Some Cases of Interest

 $\textbf{tensor} \hspace{15mm} : \hspace{15mm} \mathcal{D} \hspace{10mm} \textbf{tensor} \hspace{10mm} \textbf{of noisy measurements}$

denoising $J(\mathcal{W}) = \|\mathcal{W} - \mathcal{D}\|_F^2, \ A \ \text{and} \ \mathcal{Z} \ \text{not used}$

tensor : J(W) = 0

completion $A: (A(\mathcal{W}))_{j \in \mathbb{N}_m} = x_{i_1^j i_2^j \cdots i_N^j}, \ \mathcal{Z} \in \mathbb{R}^m$

classification : input-output pairs $\left\{ (\mathcal{X}^{(m)}, y_m) : m \in \mathbb{N}_M \right\}$

/regression $J(\mathcal{W}) = \sum_{m=1}^{M} l\left(y_m, \langle \mathcal{X}^{(m)}, \mathcal{W} \rangle\right)$, l convex loss

Tensor Completion: Image Examples

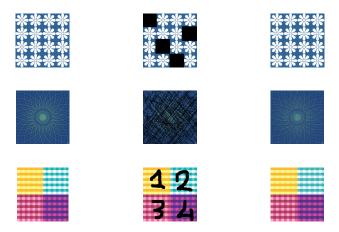


Figure: Original images (left column), the given pixels (middle column — black filled areas denote portion of the images that were removed) and reconstructed images (right column).

A Supervised Case: Classification of Aerial Views

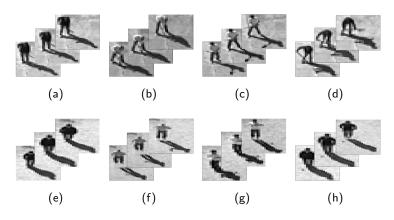


Figure: First 3 frames of low-resolution grayscale videos (3—way tensors). The first row ((a)-(d)) depicts input training patterns in the class *digging*, the second row ((e)-(h)) input training patterns in the class *jumping*.

A Supervised Case: Classification of Aerial Views (cont'd)

AUC performances on test: mean (and standard deviation) waving (I) vs waving (II) carrying VS running lin LS-SVM nuc norm lin LS-SVM nuc norm 0.81(0.15)0.83(0.14)0.82(0.11)0.60 (0.16)pointing vs standing digging vs jumping lin LS-SVM lin LS-SVM nuc norm nuc norm 0.86(0.07)0.98(0.02) $\mathbf{1}(\mathbf{0})$ 0.98(0.04)

Table: Area under the ROC curves: the tensor-based approach (nuc-norm) is compared against LS-SVMlab with linear kernel (lin LS-SVM).

Linear Versus Non-parametric Tensor-based Models

So far..

- Nuclear norm penalty to find higher order models with low multilinear ranks
- Models were still linear in the data:

$$f(\mathcal{X}_1 + \mathcal{X}_2) = \langle \mathcal{W}, \mathcal{X}_1 + \mathcal{X}_2 \rangle = \text{vec}(\mathcal{W})^{\top} \left(\text{vec}(\mathcal{X}_1) + \text{vec}(\mathcal{X}_2) \right)$$



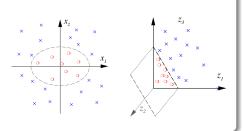
Goal

Relax linearity while exploiting the (algebraic) structure of higher order representations

A Kernel-based Framework to Tensorial Data Analysis

Kernel Methods

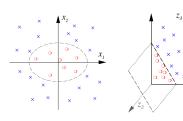
- Lead to flexible nonlinear models
- Ever use specialized kernels or ignore additional structure
- What if the number of examples is very small?



A Kernel-based Framework to Tensorial Data Analysis

Kernel Methods

- Lead to flexible nonlinear models
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A Naïve Kernel for Tensors...

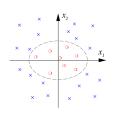
Easy to extend the Gaussian-RBF kernel to $\mathbb{R}^{I_1}\otimes\mathbb{R}^{I_2}\otimes\cdots\otimes\mathbb{R}^{I_N}$

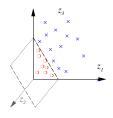
$$k(\mathcal{X}, \mathcal{Y}) = \exp\left(-\frac{1}{2\sigma^2} \|\mathcal{X} - \mathcal{Y}\|_F^2\right)$$

A Kernel-based Framework to Tensorial Data Analysis

Kernel Methods

- Lead to flexible nonlinear models
- Ever use specialized kernels or ignore additional structure
- What if the number of examples is very small?





...Does not Exploit Higher Order Representations!

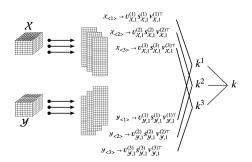
Easy to extend the Gaussian-RBF kernel to $\mathbb{R}^{I_1}\otimes\mathbb{R}^{I_2}\otimes\cdots\otimes\mathbb{R}^{I_N}$

$$k(\mathcal{X},\mathcal{Y}) = \exp\left(-\frac{1}{2\sigma^2}\|\mathcal{X} - \mathcal{Y}\|_F^2\right) = \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{vec}(\mathcal{X}) - \mathbf{vec}(\mathcal{Y})\|^2\right)$$

A Proper Kernel Framework

- optimization approach based on primal-dual formulations
- mapping performed implicitly by a tensorial kernel

Tensorial Kernel based on MLSSVD



Factor kernels k^n are based on projected Frobebius norm:

$$k^n(\mathcal{X}, \mathcal{Y}) = \exp\left(-\frac{1}{2\sigma^2} \left\| \boldsymbol{V}_{\mathcal{X}, 1}^{(n)} \boldsymbol{V}_{\mathcal{X}, 1}^{(n)\top} - \boldsymbol{V}_{\mathcal{Y}, 1}^{(n)} \boldsymbol{V}_{\mathcal{Y}, 1}^{(n)\top} \right\|_F^2\right)$$

An Illustrative Example: Classification of Sparsity Patterns

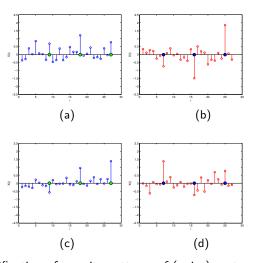


Figure: Classification of sparsity patterns of (noisy) vectors. Vectors in (a) and (c) belong to the first class whereas (b) and (d) belong to the second. The solid green (resp. solid blue) dots represent true non-zero entries (before noise corruption).

An Illustrative Example: Classification of Sparsity Patterns (cont'd)

By tensor folding turned into the classification of $3-\mathrm{rd}$ order tensors

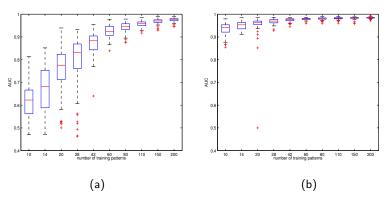


Figure: Boxplots of AUC obtained for increasing number of training patterns for the RBF-Gaussian kernel (a) and for the tensorial kernel (b).

Libras Dataset

- ► Libras = Brazilian sign language
- classes formed by 24 recordings of hand movements
- \blacktriangleright each recording is a bivariate time series (45 time instants) that is converted into $6\times2\times40$ Hankel tensor
- classification by LS-SVM with different kernels

AUC performances on test: mean (and standard deviation)

task	tensor kernel	RBF kernel	lin kernel
class 1 VS 2	0.83(0.06)	0.75(0.12)	0.77(0.13)
class 1 VS 3	0.92(0.04)	0.98(0.04)	0.94(0.09)
class 1 VS 4	1(0)	0.98(0.02)	0.95(0.07)
class 1 VS 5	1(0)	0.97(0.06)	0.91(0.12)

Concluding Remarks

- Convex multilinear estimation based on nuclear norm penalties
- ▶ A viable algorithm that makes use of first order information
- Applications in supervised and unsupervised learning
- Beyond traditional kernel methods: exploiting higher order representations

Future Research and Open Problems

- Tensor Hunting!
- Classification of Dynamical Systems
- Nuclear Norm in a primal-dual setting?

Thank You for Your Attention!

Selected References

- M. Signoretto, L. De Lathauwer and J. A. K. Suykens, Nuclear Norms for Tensors and Their Use for Convex Multilinear Estimation. Internal Report 10-186 (Submitted), ESAT-SISTA, K.U.Leuven (Leuven, Belgium), 2010, Lirias number: 270741.
- M. Signoretto, L. De Lathauwer and J. A. K. Suykens, A Kernel-based Framework to Tensorial Data Analysis, Internal Report 10-251 (Submitted), ESAT-SISTA, K.U.Leuven (Leuven, Belgium), 2010, Lirias number: 281359.
- M. Signoretto, L. De Lathauwer and J. A. K. Suykens, Convex Multilinear Estimation and Operatorial Representations, Internal Report 10-232, ESAT-SISTA, K.U.Leuven (Leuven, Belgium), 2010. NIPS Workshop: Tensors, Kernels and Machine Learning (TKML) 2010, Lirias number: 280419.
- M. Signoretto, L. De Lathauwer and J. A. K. Suykens, Kernel-based Learning from Infinite Dimensional 2-way Tensors, in ICANN 2010, part II, LNCS 6353, 2010, pp. 59-69., Lirias number: 270157.